Quantum Monte Carlo Study of an Interaction-Driven Band Insulator to Metal Transition

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We study the transitions from band insulator to metal to Mott insulator in the ionic Hubbard model on a two dimensional square lattice using determinant Quantum Monte Carlo. Evaluation of the temperature dependence of the conductivity demonstrates that the metallic region extends for a finite range of interaction values. The Mott phase at strong coupling is accompanied by antiferromagnetic (AF) order. Inclusion of these intersite correlations changes the phase diagram qualitatively compared to dynamical mean field theory.

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Introduction

Interaction effects in tight-binding models such as the Hubbard Hamiltonian have been widely studied, and understood, for their ability to drive transitions to magnetically ordered states and insulating behavior. Also extensively studied, but less well understood, is the converse phenomenon, namely the possibility that correlations can cause metallic behavior. For this latter problem, attention has focused on an Anderson insulating starting point, in which the electrons are localized by randomness. The primitive picture is that, especially away from commensurate fillings where correlations tend to localize particles in Mott insulating (MI) states, electron-electron repulsion can spread out the wave function and cause delocalization. Despite considerable effort, whether this effect actually occurs for fermionic particles in two dimensions, that is, whether metallic phases exist for disordered, interacting 2d electron systems, is not settled[1]. In an attempt to gain leverage on the problem, the phases of disordered and interacting bosonic systems have now been studied. Models such as the boson Hubbard Hamiltonian are more amenable to exact numerical studies and much is now known about the insulating, glassy, and superfluid phases, and transitions between them[2].

A somewhat simpler context in which to study the possibility of interaction driven insulator to metal transitions is to begin with a band insulating (BI) state, in which the insulating behavior is caused by a periodic external potential as opposed to a random one[3,4]. Recently, this issue has been addressed within dynamical mean field theory (DMFT) and a number of interesting conclusions emerged[5]. However, because DMFT treats only a single site (retaining, however, all the dynamical fluctuations of the self-energy which is ignored in conventional, static mean field theory) it is important to undertake complementary work which is able to retain intersite fluctuations.

In this paper, we investigate such BI-metal transitions with determinant Quantum Monte Carlo (DQMC). We study the "ionic Hubbard model":

$$\hat{\mathcal{H}} = - t \sum_{\langle lj\rangle\sigma} (c^\dagger_{j\sigma} c_{l\sigma} + c^\dagger_{l\sigma} c_{j\sigma}) + U \sum_l n_{l\uparrow} n_{l\downarrow} + \sum_l (\Delta(-1)^l - \mu)(n_{l\uparrow} + n_{l\downarrow}) \ , \quad (1)$$

where $c^\dagger_{l\sigma}(c_{l\sigma})$ are the usual fermion creation (destruction) operators for spin σ on site l, and $n_{l\sigma} = c^\dagger_{l\sigma} c_{l\sigma}$ is the number operator. t, μ and U are the electron hopping, chemical potential, and on-site interaction strength, respectively. The kinetic energy sum is over near neighbor sites $\langle lj\rangle$ on a two dimensional square lattice. $\Delta(-1)^l$ is a staggered site energy. In the noninteracting limit, $U = 0$, the effect of Δ is to produce a dispersion relation, $E(k) = \pm\sqrt{\epsilon(k)^2 + \Delta^2}$ with $\epsilon(k) = -2t[\cos k_x + \cos k_y]$, which is gapped at half-filling. A considerable amount is known concerning this model in one dimension[6], but the existence of an interaction driven metallic phase at half-filling is still unresolved even in $d = 1$. Metal-insulator transitions in a related system with *randomly* located site energies with a bimodal distribution have also been studied within DMFT[7,8].

In this letter we will use DQMC to study the role of interactions in driving a BI-metal transition in the model described by Eq. (1).

Computational Methods

DQMC[9] provides an exact numerical approach to study tight binding Hamiltonians like the Hubbard model. The partition function Z is first expressed as a path integral by discretizing the inverse temperature β. The on-site interaction is then replaced by a sum over a discrete Hubbard-Stratonovich field[10]. The resulting quadratic form in the fermion operators can be integrated analytically leaving an expression for Z in terms of a sum over all configurations of the Hubbard-Stratonovich field with a summand (Boltzmann weight) which is the product of the determinants of two matrices (one for spin up

and one for spin down). The sum is sampled stochastically using the Metropolis algorithm. The results capture correlations in the Hubbard Hamiltonian exactly since the systematic 'Trotter errors' associated with the discretization of the inverse temperature can easily be extrapolated to zero. Results must also be extrapolated to the thermodynamic limit, as we shall discuss[11].

Equal time operators such as the density and energy are measured by accumulating appropriate elements, and products of elements, of the inverse of the matrix whose determinant gives the Boltzmann weight. We will show results for the spin structure factor,

$$S(\mathbf{k}) = \sum_{l} e^{i\mathbf{k}\cdot\mathbf{l}} \ \langle \ (n_{j+l\uparrow} - n_{j+l\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \ \rangle \ ,$$

which probes magnetic order. For the conductivity, $\sigma_{\rm dc}$, We employ an approximate procedure[12] which allows $\sigma_{\rm dc}$ to be computed from the wavevector $\mathbf{q}$- and imaginary time τ-dependent current-current correlation function $\Lambda_{xx}(\mathbf{q},\tau)$ without the necessity of performing an analytic continuation[13],

$$\sigma_{\rm dc} = \frac{\beta^2}{\pi}\Lambda_{xx}(\mathbf{q}=0,\tau=\beta/2) \ .$$

Here $\beta = 1/T$, $\Lambda_{xx}(\mathbf{q},\tau) = \langle j_x(\mathbf{q},\tau)\, j_x(-\mathbf{q},0)\rangle$, and $j_x(\mathbf{q},\tau)$ the $\mathbf{q},\tau$-dependent current in the x-direction, is the Fourier transform of,

$$j_x(\ell,\tau) = i \sum_{\sigma} t_{\ell+\hat{x},\ell} \ e^{\tau H}(c^{\dagger}_{\ell+\hat{x},\sigma}c_{\ell\sigma} - c^{\dagger}_{\ell\sigma}c_{\ell+\hat{x},\sigma})e^{-\tau H} \ .$$

This approach has been extensively tested and used for the superconducting-insulator transition in the attractive Hubbard model[12], as well as for metal-insulator transitions in the repulsive model[14].

Results

We begin by showing the temperature dependence of the conductivity $\sigma_{\rm dc}$ for increasing values of the interaction strength for $\Delta = 0.5$. In Fig. 1 we see that the insulating behavior at $U = 0$, signaled by $d\sigma_{\rm dc}/dT > 0$ at low T, is changed to metallic $d\sigma_{\rm dc}/dT < 0$ at low T when $U = 1$. A further increase of the correlations to $U = 2$ weakens the metallic behavior, which is finally destroyed completely in a transition to a MI at $U = 4$. When the band gap is larger ($\Delta = 1$), the screening of the one-body potential is not sufficiently strong for $U = 1$ to cause metallic behavior, as is shown by the corresponding data set in Fig. 1. Unless otherwise mentioned, the lattice size used in the simulations is $N = 6 \times 6$ and the filling is $\rho = 1.0$ (half-filling).

In the single site ($t = 0$) limit, the ionic Hubbard model is a band insulator for $U < 2\Delta$ and a MI for $U > 2\Delta$. That is, at weak coupling and half-filling, the sites with lower energy $-\Delta$ are doubly occupied and those with higher energy $+\Delta$ are empty, with a gap to further addition of particle set by $2\Delta - U$. At strong coupling, both types of sites are singly occupied, with a 'Mott' gap to further addition of particles set by $U - 2\Delta$. At the single special value $U = 2\Delta$ correlations close the gaps[4,5]. Figure 2, which presents results for $\sigma_{\rm dc}$ for $\Delta = 0.5$, shows that when t is nonzero, this single metallic point is expanded to a finite range of U values. Interestingly, however, the largest conductivity remains near $U = 2\Delta = 1$ as one might expect from the $t = 0$ analysis. The BI to metal transition occurs at $U_{c1} \approx 0.4t$, where the change in the order of the three curves indicates a transition from $\sigma_{\rm dc}$ decreasing as β increases to $\sigma_{\rm dc}$ increasing as β

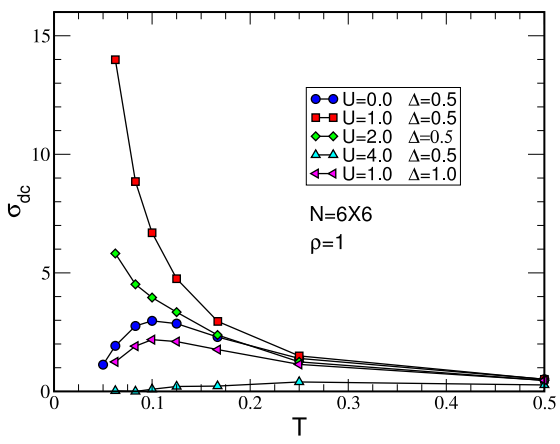

FIG. 1: The transitions, at half-filling, from a band insulator to metal to MI with increasing U are shown for periodic potential strength $\Delta = 0.5$. At U=0 the conductivity $\sigma_{\rm dc}$ goes to zero as T is lowered. However, for $U = 1t, 2t$ the system is metallic. Mott insulating behavior sets in for $U = 4t$. The lattice size is 6×6. When $\Delta = 1.0$, the band gap increases and $U = 1t$ is no longer sufficiently large to screen the one body potential and drive the system metallic.

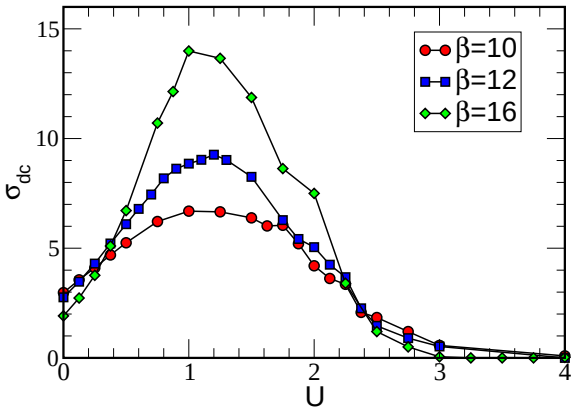

FIG. 2: The conductivity $\sigma_{\rm dc}$ at half-filling for $\Delta = 0.5$ is shown as a function of U for three different low temperatures, $\beta = 10, 12, 16$. The band-insulator to metal transition is signaled by the crossing of the curves at $U_{c1} \approx 0.4t$. At $U_{c2} \approx 2.4t$ the three curves cross again, indicating the MI transition.

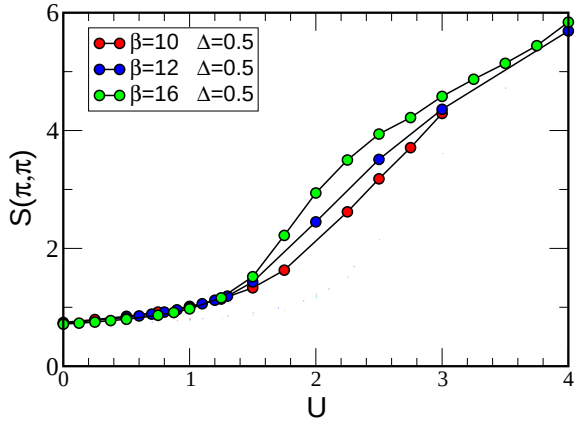

FIG. 3: The AF structure factor is shown at half-filling as a function of U for $\Delta = 0.5$ and $\beta = 10, 12, 16$.

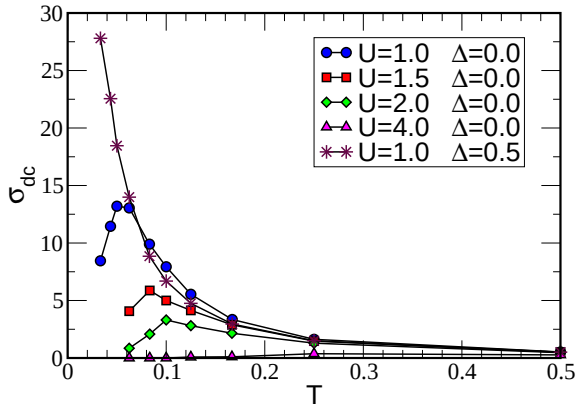

FIG. 4: The conductivity $\sigma_{\rm dc}$ is shown as a function of temperature at half-filling. When the periodic potential, and hence the non-interacting band gap, is absent ($\Delta = 0.0$) the square lattice Hubbard model is insulating for *all* U, due to nesting of the Fermi surface. We re-display data for $\Delta = 0.5, U = 1$ from Fig. 1 to emphasize the contrast between the metallic behavior there and the insulating behavior for all U when $\Delta = 0$.

increases. The metal to MI transition is at $U_{c2} \approx 2.4t$, where $\sigma_{\rm dc}$ once again decreases as β increases.

The use of DQMC to study the ionic Hubbard model allows us to examine the behavior of intersite correlations, such as the spin-spin correlations and their Fourier tranform $S(\mathbf{k})$. Fig. 3 shows results for the AF structure factor $S(\pi, \pi)$ as a function of U for $\beta = 10, 12, 16$. Comparing with Fig. 2 we see that the band insulating and metallic phases are paramagnetic, but that the transition to MI behavior is accompanied by the onset of AF order.

One way in which the inclusion of such intersite correlations changes the physics in a fundamental way is when the periodic potential is absent, that is, at $\Delta = 0$. In DMFT in the paramagnetic phase, the Hubbard model is a metal at weak coupling[15,16]. However it is well known that the $d = 2$ half-filled square lattice Hubbard model, Eq. 1, is an AF insulator at *all* U, even weak coupling.

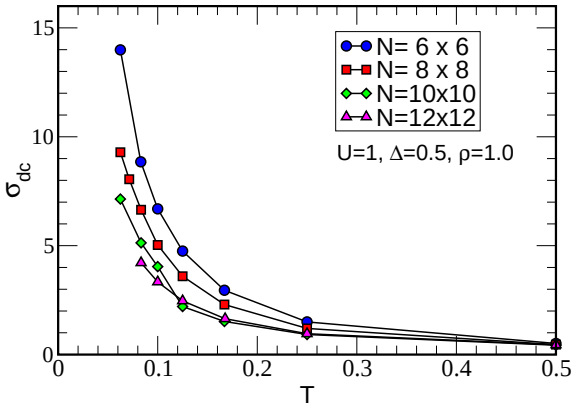

FIG. 5: The conductivity at half-filling is shown for different lattice sizes for $U = 1$, close to the point where the system is most metallic for periodic potential $\Delta = 0.5$. (See Fig. 2.) Although $\sigma_{\rm dc}$ decreases with increasing lattice sizes, the signature of metallic behavior ($d\sigma_{\rm dc}/dT < 0$) is unchanged.

Figure 4 presents our results for the conductivity which confirm this. At all U values shown, $\sigma_{\rm dc}$ ultimately decreases as T is lowered. Indeed, we have verified that the value of T where $\sigma_{\rm dc}$ has its maximum correlates well with the temperature T_* at which AF correlations begin to rise rapidly. This temperature, like the Neél temperature in the $d = 3$ Hubbard model, is a non-monotonic function of U, falling to small values both at weak ($T_* \propto t \exp(-a\sqrt{t/U})$ and at strong ($T_* \propto t^2/U$) coupling. To our knowledge, this is the first time the insulating nature of the square lattice Hubbard model at weak coupling has been shown from Quantum Monte Carlo studies of $\sigma_{\rm dc}$. It is interesting to note that while all the $\Delta = 0$ curves share a common low temperature slope $d\sigma_{\rm dc}/dT > 0$, a distinction between the origins of insulating behavior in the AF and Mott is clearly evident. At small U, $\sigma_{\rm dc}$ attains a much larger value before turning over as T is lowered than in the strong coupling Mott regime.

While DQMC allows us to look at intersite correlations and concomitant phenomena like antiferromagnetism, the method employs lattices of finite size, unlike DMFT which directly probes the thermodynamic limit. Thus, it is important to verify that the metallic phase we observe persists on larger lattices. In Fig. 5 we show results for $\sigma_{\rm dc}$ as a function of temperature in the metallic phase for lattices up to 12×12. The rise in $\sigma_{\rm dc}$ with decreasing T is seen to occur for all the lattices studied. We comment that it is not surprising that we find the lattice size has a rather substantial influence on the conductivity for these parameters, since it is known that such finite size effects are larger at weak coupling.

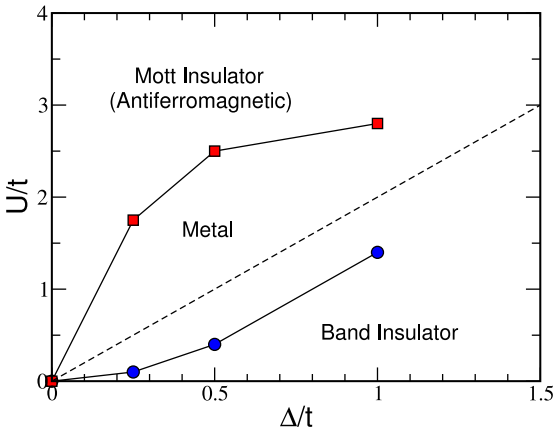

FIG. 6: The phase diagram of the ionic Hubbard model. Symbols are the result of our QMC simulations. The dashed line is the strong coupling (t=0) phase boundary between band-insulator and Mott insulator.

Conclusions

We have presented determinant Quantum Monte Carlo studies of the two-dimensional ionic Hubbard Hamiltonian which demonstrate that interactions can drive a band insulator metallic. This work complements DMFT studies by including intersite AF correlations which qualitatively alter the ground state phase diagram.

We have focused most of our results on $\Delta = 0.5$. However, we have also performed simulations sweeping U at $\Delta = 0.25$ and $\Delta = 1.00$. The emerging phase diagram is shown in Fig. 6. There are several key differences with that obtained with DMFT[5]. First, as we have emphasized, the behavior along the $\Delta = 0$ axis is significantly altered. Contrary to DMFT, the inclusion of intersite magnetic fluctuations yields an AF insulating phase for all U. Like the DMFT treatment, however, we find a metallic phase intervening between band and Mott insulators for nonzero Δ. This phase is centered roughly around the strong coupling boundary (dashed line in Fig. 6).

The sign problem prevents us from performing simulations much beyond $\Delta/t \approx 1$. However, we expect that the sign problem will become better in the limit of large Δ, where we have very widely separated bands. Related studies of the boson-Hubbard model in a "superlattice" potential, which exhibit a band-insulator to superfluid transition[3,4], show the appearance of insulating phases at half-integer fillings. These 'charge-transfer' insulators occur as a result of Mott splitting of the widely separated bands[7]. We plan to explore this possibility in the fermion case in future work.

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Note Added: A recent preprint[17] reports simulation results for the ionic Hubbard model using cluster DMFT. Like our approach, this method incorporates intersite correlations, and as found here, obtains a Mott phase along the entire $\Delta = 0$ axis of the phase diagram. A key difference is that the cluster DMFT approach suggests the intermediate phase between Mott and band insulators is a correlated 'bond ordered' insulator.

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